1171-65-185 **Paul Cazeaux*** (pcazeaux@ku.edu). *Effective modeling and simulations for atomic moiré 2D heterostructures.*

Two-dimensional crystals have been intensely investigated both experimentally and theoretically since graphene was exfoliated from graphite. Physicists have recently developed the ability to stack one layer on another with a twist angle controlled to the scale of .1° with the goal of creating two dimensional materials with desired electronic, optical, and mechanical properties. Atomic-scale lattice mismatches and twist angles create moiré patterns leading to new emergent physical phenomena shaping into a new field of twistronics. The multi-scale nature of such systems necessitates the development of new reduced order models and numerical techniques. In this talk, we will present a hierarchy of mathematical electronic structure models for the analysis and computational prediction of properties of two-dimensional layered atomic crystals in the presence of large-scale moiré patterns, focusing in particular on effective Dirac models for topological modes propagating along domain walls. (Received August 10, 2021)